



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2018 – 09:48 pm GMT

PDB ID : 2R6F  
Title : Crystal Structure of Bacillus stearothermophilus UvrA  
Authors : Inuzuka, Y.; Pakotiprapha, D.; Bowman, B.R.; Jeruzalmi, D.; Verdine, G.L.  
Deposited on : 2007-09-05  
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk31020  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk31020

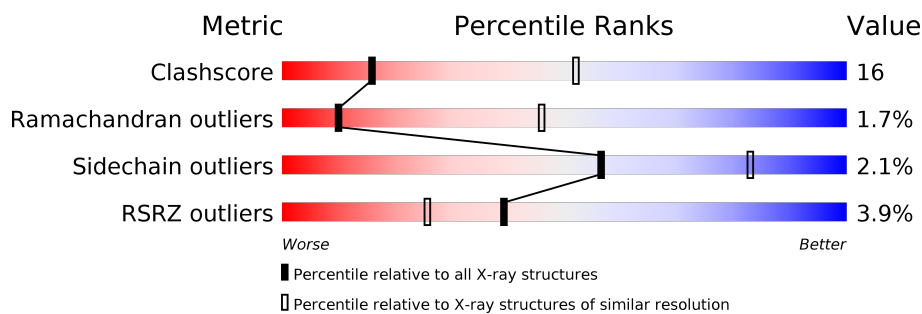
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	122126	1091 (3.20-3.20)
Ramachandran outliers	120053	1074 (3.20-3.20)
Sidechain outliers	120020	1073 (3.20-3.20)
RSRZ outliers	108989	1083 (3.22-3.18)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	972	
1	B	972	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 13986 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Excinuclease ABC subunit A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	899	Total	C	N	O	S	Se	0	0	0
			7006	4416	1231	1332	12	15			
1	B	879	Total	C	N	O	S	Se	0	0	0
			6862	4318	1212	1305	12	15			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total 3	Zn 3	0	0
3	A	3	Total 3	Zn 3	0	0

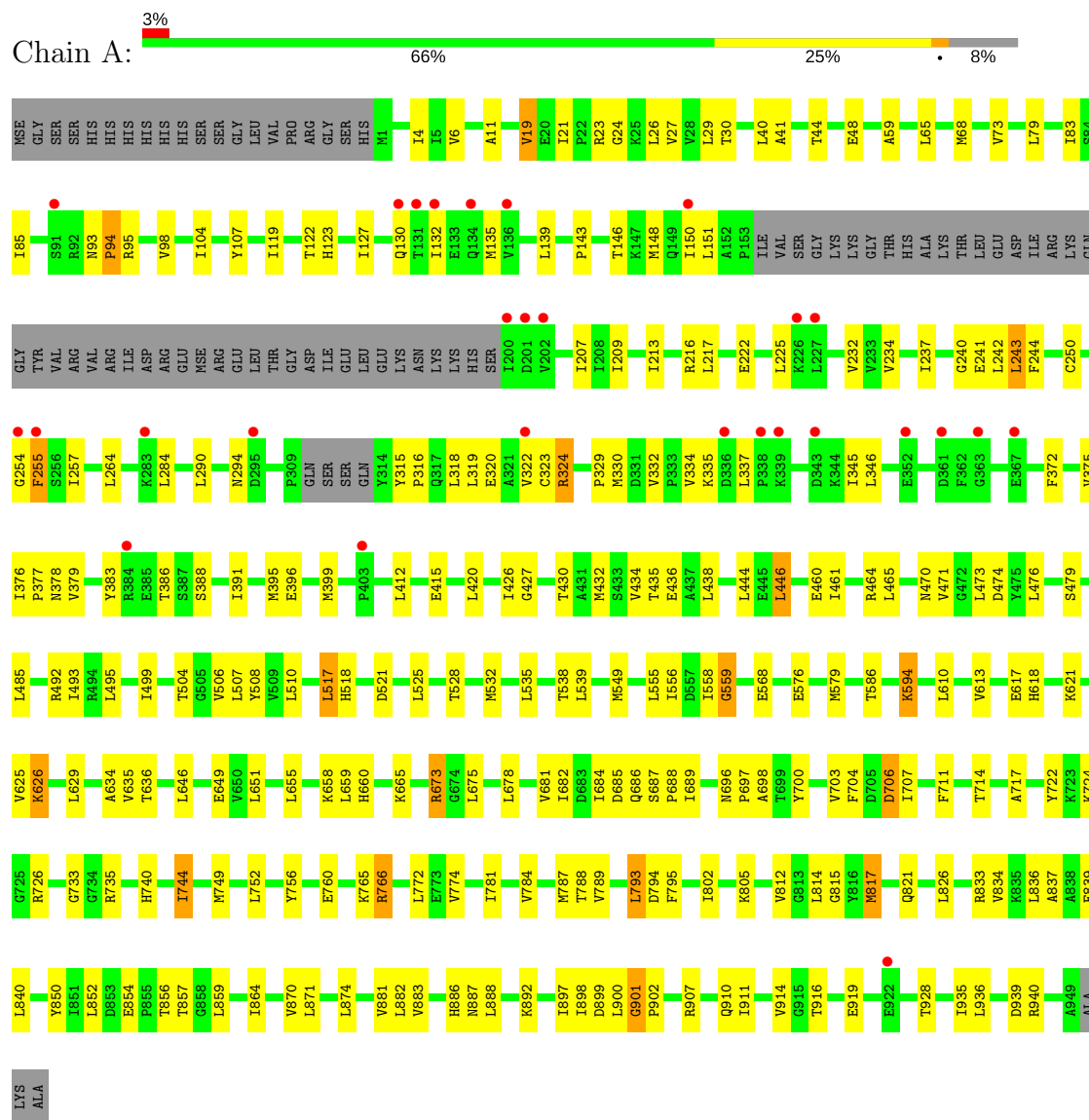
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 2	O 2	0	0
4	B	2	Total 2	O 2	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Excinuclease ABC subunit A



#### • Molecule 1: Excinuclease ABC subunit A





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.71Å 94.72Å 130.48Å 90.00° 108.80° 90.00°	Depositor
Resolution (Å)	50.00 – 3.20 33.03 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.5 (50.00-3.20) 98.6 (33.03-3.20)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.57 (at 3.18Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.253 , 0.292 0.255 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	82.0	Xtriage
Anisotropy	0.477	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 31.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	13986	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.26% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, ADP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.38	0/7114	0.63	0/9597
1	B	0.36	0/6968	0.60	0/9396
All	All	0.37	0/14082	0.61	0/18993

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7006	0	7058	241	0
1	B	6862	0	6903	200	0
2	A	54	0	24	0	0
2	B	54	0	24	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
All	All	13986	0	14009	436	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.



All (436) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:MSE:HE1	1:A:586:THR:HG21	1.30	1.07
1:A:379:VAL:HG13	1:A:395:MSE:HE3	1.34	1.06
1:B:812:VAL:HG21	1:B:837:ALA:HB2	1.36	1.06
1:A:284:LEU:HD22	1:A:399:MSE:HE3	1.39	1.05
1:A:812:VAL:HG22	1:A:836:LEU:HD12	1.44	0.98
1:B:856:THR:HG23	1:B:864:ILE:HD11	1.50	0.92
1:A:549:MSE:HE2	1:A:555:LEU:HD11	1.48	0.92
1:B:379:VAL:HA	1:B:395:MSE:HE1	1.51	0.91
1:B:871:LEU:HD12	1:B:881:VAL:HG11	1.54	0.90
1:B:549:MSE:HE1	1:B:586:THR:HG21	1.54	0.90
1:A:856:THR:HG23	1:A:864:ILE:HD11	1.54	0.89
1:B:44:THR:HG23	1:B:73:VAL:HG21	1.55	0.88
1:A:471:VAL:CG1	1:A:492:ARG:HB3	2.03	0.88
1:A:284:LEU:CD2	1:A:399:MSE:HE3	2.04	0.88
1:B:382:ARG:HB3	1:B:395:MSE:HE2	1.56	0.87
1:B:549:MSE:HE1	1:B:586:THR:CG2	2.05	0.86
1:B:6:VAL:HG13	1:B:19:VAL:HG13	1.55	0.86
1:B:6:VAL:CG1	1:B:19:VAL:HG13	2.06	0.85
1:B:379:VAL:HA	1:B:395:MSE:CE	2.06	0.84
1:A:471:VAL:HG11	1:A:492:ARG:HB3	1.61	0.83
1:A:659:LEU:HD12	1:A:681:VAL:HG23	1.61	0.82
1:A:852:LEU:HD11	1:A:871:LEU:HD11	1.61	0.82
1:A:689:ILE:HG23	1:A:700:TYR:CD2	2.16	0.80
1:A:871:LEU:HD12	1:A:881:VAL:HG11	1.63	0.80
1:A:549:MSE:HE1	1:A:586:THR:CG2	2.12	0.79
1:A:6:VAL:CG1	1:A:19:VAL:HG13	2.12	0.79
1:A:379:VAL:HG13	1:A:395:MSE:CE	2.11	0.79
1:B:812:VAL:HG13	1:B:833:ARG:HB3	1.63	0.78
1:B:634:ALA:HB3	1:B:897:ILE:HG22	1.65	0.78
1:A:379:VAL:HG22	1:A:395:MSE:HE1	1.64	0.78
1:A:104:ILE:HD13	1:A:465:LEU:HD12	1.65	0.77
1:A:290:LEU:HD11	1:A:665:LYS:HD2	1.65	0.77
1:A:264:LEU:O	1:A:264:LEU:HD23	1.85	0.77
1:A:817:MSE:HE2	1:A:821:GLN:OE1	1.85	0.76
1:A:379:VAL:HA	1:A:395:MSE:HE2	1.68	0.76
1:B:684:ILE:HD12	1:B:852:LEU:HD21	1.65	0.76
1:B:499:ILE:HD13	1:B:532:MSE:HE3	1.66	0.75
1:A:517:LEU:CD2	1:A:521:ASP:HB2	2.18	0.74
1:A:517:LEU:HD21	1:A:521:ASP:HB2	1.70	0.74
1:B:707:ILE:O	1:B:710:VAL:HG22	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:ILE:HG23	1:B:21:ILE:HB	1.70	0.74
1:B:655:LEU:HD22	1:B:675:LEU:HD13	1.68	0.73
1:A:684:ILE:HB	1:A:852:LEU:HD22	1.70	0.73
1:A:473:LEU:HD12	1:A:476:LEU:HD21	1.70	0.73
1:A:812:VAL:CG1	1:A:833:ARG:HB3	2.19	0.72
1:A:495:LEU:HD12	1:A:532:MSE:HE1	1.71	0.72
1:B:787:MSE:HE1	1:B:795:PHE:HB2	1.70	0.72
1:B:856:THR:HG21	1:B:887:ASN:HD22	1.56	0.71
1:A:499:ILE:CD1	1:A:532:MSE:HE3	2.19	0.71
1:B:68:MSE:HE1	1:B:755:VAL:HG11	1.73	0.71
1:B:471:VAL:HG11	1:B:492:ARG:HB3	1.72	0.71
1:B:888:LEU:HD13	1:B:935:ILE:HD12	1.72	0.71
1:A:207:ILE:HD11	1:A:217:LEU:HD13	1.73	0.70
1:B:684:ILE:HB	1:B:852:LEU:HD22	1.72	0.70
1:A:396:GLU:HA	1:A:399:MSE:HE2	1.73	0.70
1:A:689:ILE:HD11	1:A:834:VAL:HB	1.74	0.70
1:A:892:LYS:NZ	1:A:939:ASP:OD2	2.24	0.70
1:B:471:VAL:CG1	1:B:492:ARG:HB3	2.21	0.69
1:A:284:LEU:HD22	1:A:399:MSE:CE	2.21	0.69
1:A:788:THR:HG22	1:A:815:GLY:O	1.92	0.69
1:B:104:ILE:HD13	1:B:465:LEU:HD12	1.75	0.69
1:B:264:LEU:HD23	1:B:264:LEU:O	1.91	0.69
1:B:698:ALA:HB1	1:B:704:PHE:HB2	1.74	0.68
1:A:396:GLU:HG2	1:A:399:MSE:HE2	1.73	0.68
1:B:386:THR:HG21	1:B:391:ILE:HB	1.75	0.68
1:A:207:ILE:CD1	1:A:217:LEU:HD13	2.24	0.68
1:A:44:THR:HG23	1:A:73:VAL:HG21	1.75	0.68
1:A:83:ILE:HD12	1:A:506:VAL:HG11	1.74	0.67
1:A:6:VAL:HG13	1:A:19:VAL:HG13	1.75	0.67
1:B:485:LEU:HD13	1:B:493:ILE:HD12	1.77	0.67
1:B:379:VAL:HG13	1:B:395:MSE:HE3	1.75	0.67
1:A:781:ILE:HA	1:A:784:VAL:HG12	1.76	0.67
1:B:867:LEU:O	1:B:871:LEU:HD23	1.95	0.66
1:A:65:LEU:HD21	1:A:749:MSE:HE1	1.77	0.66
1:A:711:PHE:O	1:A:714:THR:HG22	1.96	0.65
1:A:21:ILE:HG23	1:A:27:VAL:HG21	1.77	0.65
1:B:560:PRO:HD3	1:B:570:VAL:HG22	1.78	0.65
1:A:852:LEU:CD1	1:A:871:LEU:HD11	2.27	0.64
1:A:30:THR:HG21	1:A:549:MSE:HE3	1.79	0.64
1:B:684:ILE:HD12	1:B:852:LEU:CD2	2.27	0.64
1:B:104:ILE:HD13	1:B:465:LEU:CD1	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:ILE:HD12	1:A:510:LEU:HD11	1.80	0.64
1:A:148:MSE:SE	1:A:209:ILE:HD11	2.47	0.64
1:A:4:ILE:HG23	1:A:21:ILE:HB	1.78	0.64
1:B:711:PHE:O	1:B:714:THR:HG22	1.97	0.64
1:B:655:LEU:CD2	1:B:675:LEU:HD13	2.28	0.64
1:B:112:PHE:CE2	1:B:421:VAL:HG23	2.34	0.63
1:A:332:VAL:HG11	1:A:337:LEU:HD21	1.81	0.63
1:B:508:TYR:HB2	1:B:539:LEU:HD22	1.80	0.63
1:B:888:LEU:HD13	1:B:935:ILE:CD1	2.28	0.62
1:A:495:LEU:CD1	1:A:532:MSE:HE1	2.29	0.62
1:A:396:GLU:HG2	1:A:399:MSE:CE	2.29	0.62
1:A:549:MSE:CE	1:A:555:LEU:HD11	2.27	0.62
1:B:383:TYR:CD1	1:B:399:MSE:HE1	2.34	0.62
1:A:749:MSE:HE3	1:A:752:LEU:HD12	1.81	0.61
1:A:59:ALA:HB1	1:B:91:SER:HB2	1.81	0.61
1:A:812:VAL:HG21	1:A:837:ALA:HB2	1.81	0.61
1:B:620:LEU:HD22	1:B:623:VAL:HG21	1.81	0.61
1:B:596:ILE:HD12	1:B:889:ASP:HB3	1.83	0.61
1:A:30:THR:HG21	1:A:549:MSE:CE	2.31	0.61
1:A:507:LEU:HD13	1:A:538:THR:HG23	1.83	0.61
1:B:594:LYS:HE3	1:B:594:LYS:HA	1.82	0.61
1:A:320:GLU:HA	1:A:330:MSE:HE1	1.83	0.60
1:B:559:GLY:N	1:B:568:GLU:O	2.25	0.60
1:B:897:ILE:CG1	1:B:920:VAL:HG21	2.31	0.60
1:A:499:ILE:HD11	1:A:532:MSE:HE3	1.82	0.60
1:B:213:ILE:C	1:B:213:ILE:HD12	2.22	0.60
1:B:704:PHE:HA	1:B:707:ILE:HG22	1.84	0.60
1:B:817:MSE:HE1	1:B:826:LEU:HD11	1.81	0.60
1:A:65:LEU:HD23	1:A:68:MSE:HE2	1.83	0.59
1:A:332:VAL:HG11	1:A:337:LEU:CG	2.32	0.59
1:A:634:ALA:HB3	1:A:897:ILE:HG22	1.84	0.59
1:A:610:LEU:HG	1:A:629:LEU:HD21	1.82	0.59
1:A:901:GLY:N	1:A:910:GLN:O	2.36	0.59
1:A:471:VAL:HG12	1:A:492:ARG:HB3	1.82	0.59
1:B:207:ILE:HG22	1:B:216:ARG:NH2	2.17	0.59
1:A:473:LEU:HD12	1:A:476:LEU:CD2	2.34	0.58
1:A:659:LEU:HD11	1:A:678:LEU:CD1	2.34	0.58
1:A:237:ILE:O	1:A:237:ILE:HG22	2.02	0.58
1:B:812:VAL:CG1	1:B:833:ARG:HB3	2.33	0.58
1:A:594:LYS:HA	1:A:594:LYS:HE3	1.84	0.58
1:B:646:LEU:C	1:B:646:LEU:HD23	2.23	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:LEU:CD1	1:A:493:ILE:HD12	2.34	0.58
1:A:793:LEU:HD12	1:A:794:ASP:N	2.19	0.58
1:A:383:TYR:CE1	1:A:399:MSE:HE1	2.40	0.57
1:B:549:MSE:HE2	1:B:590:LEU:HD11	1.86	0.57
1:A:613:VAL:HG21	1:A:673:ARG:NH1	2.19	0.57
1:A:104:ILE:HD13	1:A:465:LEU:CD1	2.34	0.57
1:B:689:ILE:HG23	1:B:700:TYR:CD2	2.39	0.57
1:A:684:ILE:HD12	1:A:852:LEU:HD21	1.87	0.57
1:B:684:ILE:HB	1:B:852:LEU:CD2	2.34	0.57
1:A:379:VAL:HA	1:A:395:MSE:CE	2.34	0.57
1:A:495:LEU:HD13	1:A:510:LEU:HD21	1.87	0.57
1:A:107:TYR:CZ	1:A:460:GLU:HG2	2.40	0.56
1:A:345:ILE:HG23	1:A:346:LEU:HD12	1.87	0.56
1:B:383:TYR:CE1	1:B:399:MSE:HE1	2.40	0.56
1:B:432:MSE:HE2	1:B:436:GLU:HB3	1.87	0.56
1:A:549:MSE:CE	1:A:586:THR:HG21	2.20	0.56
1:A:446:LEU:HD12	1:A:446:LEU:N	2.21	0.56
1:B:345:ILE:HG23	1:B:346:LEU:HD12	1.88	0.56
1:B:852:LEU:HD11	1:B:871:LEU:HD11	1.88	0.56
1:B:412:LEU:HD12	1:B:426:ILE:HG21	1.88	0.56
1:B:29:LEU:HD12	1:B:41:ALA:HB2	1.86	0.56
1:B:83:ILE:HD12	1:B:506:VAL:HG11	1.88	0.56
1:B:727:PHE:HB3	1:B:781:ILE:HD12	1.88	0.55
1:B:517:LEU:HD23	1:B:518:HIS:O	2.06	0.55
1:B:714:THR:HG21	1:B:774:VAL:CG1	2.36	0.55
1:A:104:ILE:HD11	1:A:464:ARG:HB3	1.87	0.55
1:B:44:THR:HG23	1:B:73:VAL:CG2	2.32	0.55
1:B:471:VAL:HG12	1:B:492:ARG:HD2	1.88	0.55
1:A:345:ILE:O	1:A:375:VAL:HG23	2.06	0.55
1:A:379:VAL:HG22	1:A:395:MSE:CE	2.35	0.55
1:B:104:ILE:HG22	1:B:108:LEU:HD23	1.86	0.55
1:A:517:LEU:HD12	1:A:525:LEU:HD22	1.88	0.55
1:A:686:GLN:NE2	1:A:857:THR:HG21	2.21	0.55
1:A:21:ILE:CG2	1:A:27:VAL:HG21	2.36	0.54
1:B:689:ILE:HD13	1:B:834:VAL:HG11	1.88	0.54
1:B:852:LEU:CD1	1:B:871:LEU:HD11	2.36	0.54
1:A:789:VAL:HB	1:A:815:GLY:HA2	1.89	0.54
1:B:150:ILE:HD12	1:B:221:LEU:HD21	1.89	0.54
1:A:625:VAL:HG22	1:A:911:ILE:HG13	1.89	0.54
1:B:396:GLU:HA	1:B:399:MSE:CE	2.37	0.54
1:A:345:ILE:HG23	1:A:346:LEU:CD1	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:LEU:H	1:A:151:LEU:HD23	1.73	0.54
1:A:319:LEU:CD2	1:A:345:ILE:HD11	2.38	0.54
1:A:470:ASN:HB3	1:A:528:THR:HG21	1.89	0.53
1:B:817:MSE:HE1	1:B:826:LEU:CD1	2.38	0.53
1:A:888:LEU:HD13	1:A:935:ILE:HD12	1.91	0.53
1:A:318:LEU:O	1:A:318:LEU:HD23	2.09	0.53
1:A:707:ILE:HD11	1:A:784:VAL:CG2	2.39	0.53
1:A:882:LEU:HD23	1:A:883:VAL:N	2.24	0.53
1:B:290:LEU:HD23	1:B:397:LYS:O	2.09	0.53
1:B:499:ILE:CD1	1:B:532:MSE:HE3	2.36	0.53
1:A:812:VAL:HG11	1:A:833:ARG:O	2.09	0.53
1:B:856:THR:HG21	1:B:887:ASN:ND2	2.20	0.53
1:A:752:LEU:CD2	1:B:57:LEU:HD13	2.38	0.53
1:A:658:LYS:CB	1:A:675:LEU:HD21	2.39	0.53
1:A:704:PHE:O	1:A:707:ILE:HG22	2.09	0.53
1:A:332:VAL:HG11	1:A:337:LEU:CD2	2.39	0.52
1:A:625:VAL:HG11	1:A:898:ILE:HD13	1.92	0.52
1:B:473:LEU:HD22	1:B:473:LEU:N	2.25	0.52
1:B:704:PHE:O	1:B:707:ILE:HG22	2.09	0.52
1:B:659:LEU:HD12	1:B:681:VAL:HG23	1.92	0.52
1:B:110:LEU:HD22	1:B:457:ILE:HG12	1.91	0.52
1:B:659:LEU:HD11	1:B:678:LEU:CD1	2.40	0.52
1:B:396:GLU:HA	1:B:399:MSE:HE3	1.91	0.52
1:B:430:THR:HG22	1:B:479:SER:HB3	1.92	0.51
1:B:549:MSE:CE	1:B:586:THR:HG21	2.35	0.51
1:B:659:LEU:HD11	1:B:678:LEU:HD13	1.92	0.51
1:A:122:THR:HG22	1:A:123:HIS:CD2	2.46	0.51
1:A:787:MSE:HE1	1:A:795:PHE:HB2	1.92	0.51
1:A:243:LEU:N	1:A:243:LEU:HD23	2.25	0.51
1:B:549:MSE:CE	1:B:555:LEU:HD11	2.41	0.51
1:A:687:SER:HB2	1:A:688:PRO:HD2	1.92	0.51
1:B:95:ARG:O	1:B:95:ARG:HG2	2.11	0.51
1:A:658:LYS:HB3	1:A:675:LEU:HD21	1.93	0.51
1:A:576:GLU:HA	1:A:579:MSE:HE2	1.93	0.51
1:A:916:THR:HG22	1:A:919:GLU:CG	2.41	0.51
1:A:24:GLY:H	1:A:538:THR:HB	1.75	0.50
1:A:332:VAL:HG11	1:A:337:LEU:HD11	1.92	0.50
1:B:646:LEU:HD23	1:B:646:LEU:O	2.11	0.50
1:A:840:LEU:HD13	1:A:840:LEU:C	2.31	0.50
1:A:684:ILE:HD12	1:A:852:LEU:CD2	2.41	0.50
1:A:722:TYR:CD2	1:A:726:ARG:HG2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:636:THR:HG23	1:A:899:ASP:HA	1.92	0.50
1:A:749:MSE:CE	1:A:752:LEU:HD12	2.42	0.50
1:B:435:THR:HG23	1:B:474:ASP:HB2	1.94	0.50
1:A:517:LEU:CD1	1:A:525:LEU:HD22	2.42	0.49
1:A:625:VAL:CG1	1:A:898:ILE:HD13	2.42	0.49
1:B:89:THR:HG23	1:B:494:ARG:CD	2.42	0.49
1:B:793:LEU:HD12	1:B:794:ASP:N	2.26	0.49
1:B:107:TYR:CZ	1:B:460:GLU:HG2	2.48	0.49
1:B:823:ALA:HA	1:B:826:LEU:HD13	1.92	0.49
1:A:44:THR:HG23	1:A:73:VAL:CG2	2.40	0.49
1:B:817:MSE:HE1	1:B:826:LEU:CG	2.42	0.49
1:A:119:ILE:HD13	1:A:420:LEU:HD21	1.95	0.49
1:B:659:LEU:CD1	1:B:681:VAL:HG23	2.42	0.49
1:B:636:THR:HG23	1:B:899:ASP:HA	1.95	0.49
1:A:504:THR:HG23	1:A:535:LEU:O	2.12	0.49
1:A:836:LEU:HD13	1:A:836:LEU:C	2.33	0.49
1:A:613:VAL:HG21	1:A:673:ARG:HH12	1.77	0.48
1:A:856:THR:HG23	1:A:864:ILE:CD1	2.36	0.48
1:A:426:ILE:HG23	1:A:427:GLY:N	2.28	0.48
1:B:412:LEU:CD1	1:B:426:ILE:HG21	2.43	0.48
1:B:86:ASP:OD2	1:B:89:THR:HG22	2.13	0.48
1:A:444:LEU:HG	1:A:446:LEU:HD11	1.95	0.48
1:A:781:ILE:O	1:A:784:VAL:HG12	2.13	0.48
1:B:722:TYR:CD2	1:B:726:ARG:HG2	2.48	0.48
1:B:840:LEU:C	1:B:840:LEU:HD13	2.33	0.48
1:A:435:THR:HG23	1:A:474:ASP:O	2.13	0.48
1:A:698:ALA:HB1	1:A:704:PHE:HB2	1.95	0.48
1:B:290:LEU:HD11	1:B:665:LYS:HD2	1.94	0.48
1:A:714:THR:HG21	1:A:774:VAL:CG1	2.43	0.48
1:A:870:VAL:O	1:A:874:LEU:HD23	2.13	0.48
1:B:812:VAL:CG2	1:B:837:ALA:HB2	2.25	0.48
1:B:29:LEU:CD1	1:B:41:ALA:HB2	2.43	0.48
1:A:323:CYS:O	1:A:324:ARG:C	2.52	0.48
1:A:130:GLN:O	1:A:135:MSE:HE3	2.13	0.47
1:A:432:MSE:HE2	1:A:436:GLU:HB3	1.95	0.47
1:B:704:PHE:HA	1:B:707:ILE:CG2	2.43	0.47
1:A:237:ILE:CG2	1:A:237:ILE:O	2.62	0.47
1:A:812:VAL:HG13	1:A:833:ARG:HB3	1.94	0.47
1:A:856:THR:HG21	1:A:887:ASN:HD22	1.78	0.47
1:A:636:THR:HG21	1:A:928:THR:HG21	1.95	0.47
1:B:613:VAL:HG21	1:B:673:ARG:HH12	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:707:ILE:HD11	1:A:784:VAL:HG21	1.95	0.47
1:B:379:VAL:HG13	1:B:395:MSE:CE	2.42	0.47
1:B:872:HIS:NE2	1:B:893:THR:HG22	2.30	0.47
1:B:94:PRO:O	1:B:95:ARG:HB3	2.13	0.47
1:A:383:TYR:CZ	1:A:399:MSE:HE1	2.50	0.47
1:A:871:LEU:HD12	1:A:881:VAL:CG1	2.40	0.47
1:A:139:LEU:HD22	1:A:148:MSE:SE	2.64	0.47
1:B:24:GLY:H	1:B:538:THR:HB	1.80	0.47
1:B:707:ILE:HD11	1:B:796:PHE:CZ	2.49	0.47
1:A:499:ILE:HD13	1:A:532:MSE:HE3	1.96	0.47
1:B:471:VAL:HG12	1:B:471:VAL:O	2.14	0.47
1:B:857:THR:O	1:B:857:THR:HG23	2.14	0.47
1:A:257:ILE:HD13	1:A:415:GLU:HB2	1.96	0.47
1:A:555:LEU:C	1:A:555:LEU:HD23	2.35	0.47
1:A:294:ASN:HD21	1:A:658:LYS:NZ	2.13	0.47
1:A:856:THR:HG21	1:A:887:ASN:ND2	2.30	0.47
1:A:319:LEU:HD21	1:A:345:ILE:HD11	1.97	0.47
1:B:625:VAL:HG22	1:B:626:LYS:H	1.80	0.47
1:B:655:LEU:HD22	1:B:675:LEU:CD1	2.40	0.47
1:B:684:ILE:CD1	1:B:836:LEU:HD23	2.45	0.47
1:B:765:LYS:O	1:B:766:ARG:HB2	2.14	0.47
1:B:897:ILE:HG13	1:B:920:VAL:HG21	1.96	0.46
1:A:812:VAL:HG22	1:A:836:LEU:CD1	2.32	0.46
1:B:112:PHE:CD2	1:B:421:VAL:HG23	2.50	0.46
1:B:21:ILE:HG23	1:B:27:VAL:HG21	1.96	0.46
1:A:430:THR:HG22	1:A:479:SER:HB3	1.98	0.46
1:A:518:HIS:HA	1:A:886:HIS:ND1	2.30	0.46
1:B:434:VAL:HB	1:B:474:ASP:HA	1.98	0.46
1:A:213:ILE:C	1:A:213:ILE:HD12	2.35	0.46
1:B:625:VAL:HG22	1:B:626:LYS:N	2.30	0.46
1:B:696:ASN:HB2	1:B:697:PRO:HD2	1.98	0.46
1:B:207:ILE:CD1	1:B:217:LEU:HD13	2.46	0.46
1:B:517:LEU:HD21	1:B:521:ASP:HB2	1.97	0.46
1:A:684:ILE:CD1	1:A:836:LEU:HD23	2.45	0.46
1:B:613:VAL:HG21	1:B:673:ARG:NH1	2.30	0.46
1:A:704:PHE:HA	1:A:707:ILE:HG22	1.98	0.46
1:B:412:LEU:HD12	1:B:426:ILE:CG2	2.46	0.46
1:A:696:ASN:O	1:A:697:PRO:C	2.53	0.46
1:A:850:TYR:CE1	1:A:874:LEU:HD12	2.50	0.46
1:B:207:ILE:HG22	1:B:216:ARG:CZ	2.46	0.46
1:B:781:ILE:HA	1:B:784:VAL:HG12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:788:THR:CG2	1:A:815:GLY:O	2.63	0.46
1:B:345:ILE:HG23	1:B:346:LEU:CD1	2.46	0.46
1:B:555:LEU:HD22	1:B:578:VAL:HG11	1.97	0.46
1:A:626:LYS:HE3	1:A:626:LYS:H	1.81	0.46
1:B:689:ILE:HD12	1:B:826:LEU:HD22	1.98	0.46
1:B:812:VAL:HG12	1:B:814:LEU:HD13	1.97	0.46
1:B:689:ILE:HD11	1:B:834:VAL:HB	1.98	0.46
1:A:127:ILE:HG22	1:A:250:CYS:HA	1.98	0.45
1:A:660:HIS:HE1	1:A:681:VAL:H	1.62	0.45
1:B:900:LEU:HD12	1:B:911:ILE:HD13	1.98	0.45
1:A:765:LYS:O	1:A:766:ARG:HB2	2.16	0.45
1:A:682:ILE:HG21	1:A:839:GLU:HG2	1.98	0.45
1:A:714:THR:HG23	1:A:717:ALA:H	1.81	0.45
1:B:635:VAL:HG21	1:B:647:VAL:CG2	2.46	0.45
1:A:461:ILE:O	1:A:465:LEU:HD13	2.16	0.45
1:B:107:TYR:CE2	1:B:460:GLU:HG2	2.51	0.45
1:B:461:ILE:O	1:B:465:LEU:HD13	2.17	0.45
1:B:625:VAL:HG21	1:B:898:ILE:HD13	1.99	0.45
1:B:812:VAL:CG1	1:B:814:LEU:HD13	2.46	0.45
1:A:508:TYR:HB2	1:A:539:LEU:HD22	1.98	0.45
1:B:612:VAL:CG2	1:B:625:VAL:HG12	2.47	0.45
1:B:687:SER:HB2	1:B:688:PRO:HD2	1.98	0.45
1:A:517:LEU:HD21	1:A:521:ASP:CB	2.44	0.45
1:A:655:LEU:HB3	1:A:681:VAL:HG21	1.99	0.45
1:B:471:VAL:HG12	1:B:492:ARG:HB3	1.95	0.45
1:B:635:VAL:HG21	1:B:647:VAL:HG22	1.99	0.45
1:A:499:ILE:CD1	1:A:532:MSE:CE	2.94	0.45
1:A:651:LEU:HD11	1:A:655:LEU:HD11	1.97	0.45
1:B:48:GLU:HB3	1:B:79:LEU:HD11	1.97	0.45
1:B:526:ILE:CD1	1:B:548:THR:HG23	2.47	0.45
1:B:678:LEU:HA	1:B:847:ARG:HB3	1.99	0.45
1:A:207:ILE:HG22	1:A:216:ARG:NH1	2.32	0.45
1:A:635:VAL:CG2	1:A:882:LEU:HD21	2.47	0.45
1:A:29:LEU:HD23	1:A:556:ILE:HB	1.99	0.44
1:B:651:LEU:HD11	1:B:655:LEU:HD11	1.99	0.44
1:A:817:MSE:HE1	1:A:826:LEU:HG	1.98	0.44
1:A:558:ILE:O	1:A:559:GLY:O	2.35	0.44
1:A:150:ILE:CD1	1:A:234:VAL:HG22	2.47	0.44
1:A:65:LEU:CD2	1:A:749:MSE:HE1	2.46	0.44
1:B:386:THR:HG21	1:B:391:ILE:CB	2.44	0.44
1:A:703:VAL:HG22	1:A:805:LYS:CB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:716:GLU:HB3	1:B:774:VAL:HG22	1.99	0.44
1:B:897:ILE:HD11	1:B:920:VAL:HG11	1.98	0.44
1:A:225:LEU:HD21	1:A:232:VAL:HG12	1.98	0.44
1:A:329:PRO:HG2	1:A:332:VAL:HG21	2.00	0.44
1:A:508:TYR:HB2	1:A:539:LEU:CD2	2.48	0.44
1:B:127:ILE:HG22	1:B:250:CYS:HA	2.00	0.44
1:A:143:PRO:HG2	1:A:146:THR:HG21	2.00	0.44
1:A:207:ILE:HG22	1:A:216:ARG:CZ	2.48	0.44
1:B:472:GLY:C	1:B:473:LEU:HD22	2.38	0.44
1:B:871:LEU:HD12	1:B:881:VAL:CG1	2.38	0.44
1:A:94:PRO:O	1:A:95:ARG:HB3	2.18	0.43
1:B:425:HIS:CE1	1:B:428:GLU:HG3	2.53	0.43
1:B:585:LEU:HD23	1:B:585:LEU:O	2.17	0.43
1:B:345:ILE:O	1:B:375:VAL:HG23	2.18	0.43
1:A:23:ARG:HH22	1:B:504:THR:HG21	1.83	0.43
1:A:635:VAL:HG23	1:A:882:LEU:HD21	2.01	0.43
1:A:703:VAL:HG22	1:A:805:LYS:HB2	2.01	0.43
1:B:726:ARG:HG3	1:B:771:THR:HG23	2.00	0.43
1:B:833:ARG:CZ	1:B:859:LEU:HD21	2.48	0.43
1:A:412:LEU:CD1	1:A:426:ILE:HG21	2.49	0.43
1:A:434:VAL:HB	1:A:474:ASP:HA	2.00	0.43
1:A:655:LEU:HD23	1:A:675:LEU:CD1	2.48	0.43
1:A:840:LEU:HD21	1:A:870:VAL:HG13	2.01	0.43
1:A:332:VAL:HG11	1:A:337:LEU:CD1	2.49	0.43
1:B:264:LEU:HD23	1:B:416:SER:OG	2.18	0.43
1:B:817:MSE:HE1	1:B:826:LEU:HG	1.99	0.43
1:A:315:TYR:N	1:A:316:PRO:CD	2.82	0.43
1:A:706:ASP:HB2	1:A:802:ILE:HD13	2.00	0.43
1:A:857:THR:O	1:A:857:THR:HG23	2.18	0.43
1:B:315:TYR:N	1:B:316:PRO:CD	2.81	0.43
1:A:376:ILE:HB	1:A:377:PRO:HD3	2.00	0.43
1:A:485:LEU:HD13	1:A:493:ILE:HD12	2.00	0.43
1:A:646:LEU:HD12	1:A:900:LEU:HD11	2.00	0.43
1:A:856:THR:O	1:A:857:THR:C	2.57	0.43
1:B:471:VAL:CG1	1:B:492:ARG:HD2	2.48	0.43
1:B:652:TYR:CE2	1:B:683:ASP:HB2	2.53	0.43
1:B:717:ALA:O	1:B:722:TYR:N	2.51	0.43
1:B:821:GLN:HA	1:B:822:PRO:HD3	1.90	0.43
1:A:378:ASN:OD1	1:A:378:ASN:C	2.56	0.43
1:A:916:THR:HG22	1:A:919:GLU:HG3	2.00	0.43
1:A:254:GLY:O	1:A:255:PHE:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:854:GLU:O	1:A:857:THR:HG22	2.18	0.43
1:B:549:MSE:HE2	1:B:555:LEU:HD11	1.99	0.43
1:A:781:ILE:CA	1:A:784:VAL:HG12	2.48	0.42
1:B:473:LEU:HD21	1:B:492:ARG:HE	1.84	0.42
1:B:781:ILE:O	1:B:784:VAL:HG12	2.18	0.42
1:A:332:VAL:HG11	1:A:337:LEU:HG	2.01	0.42
1:A:504:THR:HG22	1:B:23:ARG:HH12	1.84	0.42
1:A:735:ARG:NH1	1:A:740:HIS:HA	2.34	0.42
1:A:902:PRO:O	1:A:907:ARG:O	2.36	0.42
1:A:752:LEU:HD21	1:B:57:LEU:HD13	2.01	0.42
1:A:936:LEU:HD22	1:A:940:ARG:NH2	2.33	0.42
1:B:457:ILE:H	1:B:457:ILE:HD12	1.84	0.42
1:A:744:ILE:HG21	1:A:756:TYR:HB3	2.01	0.42
1:B:379:VAL:CA	1:B:395:MSE:CE	2.89	0.42
1:A:240:GLY:O	1:A:242:LEU:N	2.53	0.42
1:B:357:ARG:HH21	1:B:365:VAL:HG21	1.85	0.42
1:B:856:THR:CG2	1:B:864:ILE:HD11	2.36	0.42
1:A:65:LEU:HD21	1:A:749:MSE:CE	2.47	0.42
1:A:704:PHE:HA	1:A:707:ILE:CG2	2.49	0.42
1:B:694:ARG:HA	1:B:729:PHE:HE2	1.85	0.42
1:B:457:ILE:HD12	1:B:457:ILE:N	2.35	0.41
1:B:812:VAL:HG21	1:B:837:ALA:CB	2.27	0.41
1:A:685:ASP:OD1	1:A:686:GLN:N	2.53	0.41
1:B:329:PRO:HB2	1:B:332:VAL:HG23	2.02	0.41
1:B:589:TYR:OH	1:B:862:ASP:OD1	2.29	0.41
1:B:432:MSE:HB2	1:B:437:ALA:HB2	2.02	0.41
1:B:22:PRO:HG3	1:B:554:TYR:CG	2.55	0.41
1:A:322:VAL:HG21	1:A:372:PHE:CZ	2.55	0.41
1:A:386:THR:HG22	1:A:388:SER:N	2.34	0.41
1:A:833:ARG:CZ	1:A:859:LEU:HD21	2.50	0.41
1:B:379:VAL:CG1	1:B:395:MSE:HE3	2.47	0.41
1:A:151:LEU:N	1:A:151:LEU:HD23	2.34	0.41
1:A:243:LEU:N	1:A:243:LEU:CD2	2.84	0.41
1:A:684:ILE:HB	1:A:852:LEU:CD2	2.45	0.41
1:A:900:LEU:O	1:A:901:GLY:O	2.39	0.41
1:A:93:ASN:HA	1:A:94:PRO:HD2	1.83	0.41
1:A:132:ILE:HD13	1:A:222:GLU:HB2	2.03	0.41
1:A:839:GLU:O	1:A:840:LEU:C	2.59	0.41
1:A:29:LEU:CD1	1:A:41:ALA:HB2	2.51	0.41
1:A:659:LEU:CD1	1:A:681:VAL:HG23	2.42	0.41
1:B:19:VAL:HG11	1:B:40:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:636:THR:HG23	1:A:899:ASP:OD2	2.20	0.41
1:A:438:LEU:HD13	1:A:465:LEU:CB	2.51	0.41
1:A:655:LEU:HD23	1:A:675:LEU:HD13	2.03	0.41
1:A:812:VAL:CG1	1:A:812:VAL:O	2.69	0.41
1:B:342:LEU:HA	1:B:345:ILE:HG22	2.03	0.41
1:B:372:PHE:CE2	1:B:374:GLY:HA2	2.56	0.41
1:B:575:PRO:O	1:B:579:MSE:HB2	2.20	0.41
1:B:598:ILE:HG23	1:B:602:ARG:NH1	2.36	0.41
1:A:386:THR:HG21	1:A:391:ILE:HB	2.03	0.40
1:A:559:GLY:N	1:A:568:GLU:O	2.33	0.40
1:A:911:ILE:HG21	1:A:914:VAL:HG13	2.03	0.40
1:A:98:VAL:HG21	1:A:476:LEU:HD13	2.03	0.40
1:B:473:LEU:N	1:B:473:LEU:CD2	2.83	0.40
1:B:817:MSE:HE2	1:B:821:GLN:HB3	2.03	0.40
1:A:812:VAL:HG21	1:A:837:ALA:CB	2.49	0.40
1:A:48:GLU:HB3	1:A:79:LEU:HD11	2.03	0.40
1:B:434:VAL:HG23	1:B:476:LEU:O	2.22	0.40
1:B:714:THR:HG23	1:B:717:ALA:H	1.87	0.40
1:B:747:ILE:HG22	1:B:755:VAL:O	2.22	0.40
1:A:329:PRO:HG2	1:A:332:VAL:CG2	2.50	0.40
1:B:379:VAL:O	1:B:395:MSE:HE3	2.21	0.40
1:B:104:ILE:CD1	1:B:465:LEU:HD12	2.49	0.40
1:B:678:LEU:HD12	1:B:678:LEU:O	2.22	0.40
1:A:386:THR:HG22	1:A:388:SER:H	1.87	0.40
1:A:470:ASN:CB	1:A:528:THR:HG21	2.51	0.40
1:B:549:MSE:HE3	1:B:555:LEU:HD11	2.02	0.40
1:B:703:VAL:HG22	1:B:805:LYS:CB	2.52	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	893/972 (92%)	823 (92%)	56 (6%)	14 (2%)	11	47
1	B	873/972 (90%)	787 (90%)	70 (8%)	16 (2%)	9	45
All	All	1766/1944 (91%)	1610 (91%)	126 (7%)	30 (2%)	10	46

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	559	GLY
1	A	617	GLU
1	A	901	GLY
1	B	11	ALA
1	B	94	PRO
1	B	258	GLY
1	B	559	GLY
1	B	617	GLU
1	B	901	GLY
1	A	11	ALA
1	A	241	GLU
1	A	255	PHE
1	A	334	VAL
1	B	76	ILE
1	B	257	ILE
1	B	277	CYS
1	B	733	GLY
1	B	814	LEU
1	A	94	PRO
1	A	733	GLY
1	A	814	LEU
1	B	372	PHE
1	A	324	ARG
1	B	293	PRO
1	A	724	LYS
1	B	309	PRO
1	B	618	HIS
1	A	618	HIS
1	A	766	ARG
1	B	8	GLY

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar

resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	755/801 (94%)	736 (98%)	19 (2%)	50	80
1	B	739/801 (92%)	727 (98%)	12 (2%)	65	87
All	All	1494/1602 (93%)	1463 (98%)	31 (2%)	56	83

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	VAL
1	A	26	LEU
1	A	40	LEU
1	A	243	LEU
1	A	244	PHE
1	A	335	LYS
1	A	446	LEU
1	A	517	LEU
1	A	594	LYS
1	A	621	LYS
1	A	626	LYS
1	A	649	GLU
1	A	673	ARG
1	A	706	ASP
1	A	744	ILE
1	A	760	GLU
1	A	772	LEU
1	A	793	LEU
1	A	817	MSE
1	B	19	VAL
1	B	26	LEU
1	B	284	LEU
1	B	335	LYS
1	B	464	ARG
1	B	476	LEU
1	B	538	THR
1	B	594	LYS
1	B	626	LYS
1	B	673	ARG
1	B	760	GLU
1	B	848	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	248	HIS
1	A	294	ASN
1	A	498	GLN
1	A	657	GLN
1	A	660	HIS
1	A	763	HIS
1	B	302	HIS
1	B	669	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	ADP	A	1000	-	25,29,29	1.08	2 (8%)	25,45,45	1.93	3 (12%)
2	ADP	A	1001	-	25,29,29	1.04	2 (8%)	25,45,45	1.93	5 (20%)
2	ADP	B	1002	-	25,29,29	1.02	2 (8%)	25,45,45	2.09	4 (16%)
2	ADP	B	1003	-	25,29,29	1.02	1 (4%)	25,45,45	1.91	5 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	1000	-	-	0/12/32/32	0/3/3/3
2	ADP	A	1001	-	-	0/12/32/32	0/3/3/3
2	ADP	B	1002	-	-	0/12/32/32	0/3/3/3
2	ADP	B	1003	-	-	0/12/32/32	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	ADP	C8-N9	-2.02	1.34	1.36
2	B	1002	ADP	C2-N3	2.02	1.35	1.32
2	A	1000	ADP	O4'-C1'	2.14	1.44	1.41
2	B	1002	ADP	C5-C4	2.77	1.46	1.40
2	A	1000	ADP	C5-C4	2.80	1.46	1.40
2	B	1003	ADP	C5-C4	2.86	1.46	1.40
2	A	1001	ADP	C5-C4	2.97	1.47	1.40

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1000	ADP	N3-C2-N1	-7.43	122.50	128.86
2	B	1003	ADP	N3-C2-N1	-7.40	122.53	128.86
2	A	1001	ADP	N3-C2-N1	-7.24	122.67	128.86
2	B	1002	ADP	N3-C2-N1	-7.21	122.69	128.86
2	B	1002	ADP	PA-O3A-PB	-4.46	117.64	132.63
2	B	1002	ADP	C4-C5-N7	-3.26	106.26	109.41
2	A	1000	ADP	PA-O3A-PB	-3.20	121.86	132.63
2	A	1001	ADP	PA-O3A-PB	-3.00	122.53	132.63
2	A	1001	ADP	C4-C5-N7	-2.97	106.54	109.41
2	A	1000	ADP	C4-C5-N7	-2.61	106.89	109.41
2	B	1003	ADP	C4-C5-N7	-2.29	107.20	109.41
2	B	1003	ADP	PA-O3A-PB	-2.27	125.00	132.63
2	B	1003	ADP	O3B-PB-O2B	2.03	115.60	107.59
2	B	1002	ADP	O3B-PB-O2B	2.07	115.78	107.59
2	A	1001	ADP	C2-N1-C6	2.08	122.29	118.75
2	B	1003	ADP	C2-N1-C6	2.11	122.33	118.75
2	A	1001	ADP	O3B-PB-O2B	2.17	116.16	107.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	884/972 (90%)	0.04	28 (3%)	47 31	57, 86, 148, 198	0
1	B	864/972 (88%)	0.17	41 (4%)	31 19	66, 103, 156, 185	0
All	All	1748/1944 (89%)	0.10	69 (3%)	39 26	57, 94, 155, 198	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	130	GLN	6.7
1	B	221	LEU	5.1
1	B	149	GLN	5.0
1	B	132	ILE	4.9
1	B	727	PHE	4.8
1	B	206	ARG	4.8
1	B	142	TYR	4.7
1	B	136	VAL	4.4
1	B	139	LEU	4.4
1	A	322	VAL	4.1
1	B	729	PHE	4.0
1	B	711	PHE	4.0
1	B	138	ARG	3.8
1	A	254	GLY	3.7
1	B	229	ASP	3.7
1	A	361	ASP	3.6
1	B	140	LEU	3.5
1	A	283	LYS	3.3
1	A	336	ASP	3.3
1	B	205	ASP	3.1
1	B	227	LEU	3.1
1	B	661	ARG	3.1
1	A	227	LEU	3.1
1	A	226	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	131	THR	3.0
1	B	151	LEU	3.0
1	B	796	PHE	2.9
1	A	130	GLN	2.9
1	A	136	VAL	2.9
1	B	663	LYS	2.8
1	B	129	SER	2.8
1	A	352	GLU	2.8
1	B	228	ALA	2.7
1	B	336	ASP	2.6
1	A	255	PHE	2.6
1	B	751	PHE	2.6
1	B	143	PRO	2.6
1	A	202	VAL	2.5
1	B	748	GLU	2.5
1	B	150	ILE	2.5
1	B	217	LEU	2.5
1	B	754	ASP	2.5
1	A	343	ASP	2.4
1	B	311	SER	2.4
1	B	224	ALA	2.4
1	A	200	ILE	2.4
1	B	207	ILE	2.4
1	B	719	VAL	2.4
1	A	339	LYS	2.3
1	B	398	TYR	2.3
1	A	922	GLU	2.3
1	A	295	ASP	2.2
1	A	91	SER	2.2
1	B	704	PHE	2.2
1	A	201	ASP	2.2
1	B	707	ILE	2.2
1	A	403	PRO	2.2
1	A	338	PRO	2.1
1	A	132	ILE	2.1
1	A	367	GLU	2.1
1	B	225	LEU	2.1
1	B	750	HIS	2.1
1	A	134	GLN	2.1
1	A	363	GLY	2.1
1	A	150	ILE	2.0
1	B	397	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	384	ARG	2.0
1	B	400	ALA	2.0
1	B	785	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	ZN	A	1004	1/1	0.88	0.09	96,96,96,96	0
2	ADP	A	1000	27/27	0.92	0.21	59,65,66,67	0
3	ZN	B	1008	1/1	0.92	0.05	103,103,103,103	0
2	ADP	B	1002	27/27	0.93	0.18	75,81,82,82	0
2	ADP	B	1003	27/27	0.93	0.17	68,71,72,72	0
2	ADP	A	1001	27/27	0.95	0.17	57,68,70,70	0
3	ZN	A	1006	1/1	0.96	0.11	89,89,89,89	0
3	ZN	B	1007	1/1	0.97	0.10	94,94,94,94	0
3	ZN	B	1009	1/1	0.98	0.17	99,99,99,99	0
3	ZN	A	1005	1/1	0.99	0.05	92,92,92,92	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.